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Comparison of Three Ozone Models: Urban Airshed, City-Specific EKMA and Proportional Rollback

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16. ABSTRACT

The results of using three different types of models to assess the potential effectiveness of ozone control strategies are described. Data collected during the RAPS program conducted in St. Louis were used to develop inputs for a complex photochemical air quality simulation model. The model was used to simulate a number of control strategies to establish their potential for lowering ozone levels. These strategies were replicated with two simpler models - City-specific and Rollback. The results obtained with the simpler models were then compared to those found with the more complex model. Neither of the simpler models agreed with the complex under all conditions. However, in estimating the degree of control necessary to reduce peak ozone to the level of the national standard, the differences between the complex model and City-specific EKMA were usually less than 10%. Differences between Rollback and the complex model were usually less than 20%.

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by

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March 1982

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PREFACE

The Urban Airshed Model Simulations described in this report were conducted by the Source Receptor Analysis Branch (SRAB) of the Office of Air Quality Planning and Standards in EPA. The author gratefully acknowledges the invaluable assistance of Conrad Newberry and Gerald Moss of SRAB in providing the Airshed Modeling information needed to conduct this project. Special thanks are extended to Dr. Edwin L. Meyer and Dr. Henry S. Cole for their valuable comments and suggestions, and to Mrs. Carole Mask for typing and editing.

EXECUTIVE SUMMARY

The purpose of this study has been to assess the validity of City-specific EKMA and Rollback by comparing their predictions of control strategy effectiveness with those of a more complex Eulerian Photochemical Air Quality Simulation Model (PAQSM). In this type of analysis, the complex model is assumed to provide the best estimates of control strategy effectiveness and is used to simulate a number of potential control scenarios. The results are then used to measure the performance of the simple models. An important limitation of this study is that no absolute assurance exists that the PAQSM provides accurate estimates of the effects of potential control programs. Such a limitation cannot be overcome until the PAQSM is validated both in a pre-control and a post-control situation. However, to minimize the possibilities of errors in the model inputs, the PAQSM should reproduce existing ozone patterns reasonably well (i.e., observations and model projections should agree within some acceptable error bound).

In this particular study, a complex PAQSM, developed by Systems Applications, Incorporated, the Urban Airshed Model, was applied to the St. Louis Metropolitan Area using the 1976 Regional Air Pollution Study (RAPS) data base. The model was used to simulate ozone patterns observed on specific days in the RAPS, and then used to simulate changes in emission levels from the base period. The effects were noted, then used to assess the ability of the simple models to replicate these results. The major findings arising from the study and their implications are listed below:

Finding: Neither Rollback nor City-specific EKMA reproduces Airshed Model results under <u>all</u> conditions.

Implication: In particular circumstances, the use of simple models can lead to results which are different from those found with the Airshed Model. However, neither simple model was found to be consistently overly or underly conservative in the predictions of control program effectiveness.

Finding: In estimating the level of control needed to reduce peak ozone to 120 ppb, the difference in control levels obtained with City-specific EKMA and those found with the Urban Airshed Model was usually within about ±10%. Most often, City-specific EKMA control estimates were lower than the Airshed Model.

Implication: Several investigations have suggested that City-specific EKMA is overly conservative in its predictions of emission reductions necessary to achieve the ozone standard. Airshed Model results suggest that this hypothesis is not correct.

Finding: Rollback predictions of controls needed to reduce peak ozone levels to 120 ppb agreed with Airshed in some cases, but gave substantially lower controls in others.

Implication: The rollback model may underpredict control requirements in some cases. Airshed Model results imply that Rollback may underpredict, in some cases, by as much as 20% (e.g, 40% control versus 60%). The tendency to underpredict is most prevalent when relatively high (e.g., 13:1) HC/NO_x ratios prevail.

Finding: Airshed Model predictions of peak ozone observed during the RAPS were usually within ±30% of observations. However, the magnitude, location and timing of the regionwide predicted peaks often differed from the observed peaks, sometimes substantially.

Implication: While the above results are not surprising, they indicate that procedures to account for these discrepancies in a regulatory application of a PAQSM need to be developed if PAQSMs are to reach their potential for spatial and temporal resolution.

Finding: The Airshed Model predictions of control strategy effectiveness varied from day to day (i.e., strategies may be more effective under some meteorological conditions than others). This same finding applied to City-specific EKMA, and to a much lesser extent, Rollback.

Implication: As a result of differing control effectivess predictions, procedures for relating Airshed Model results to the statistical form of the ozone standard are needed. Modeling a single day to estimate the controls needed is not sufficient. At a minimum, several days representing different meteorological conditions corresponding to high ozone levels need to be modeled.

Finding: When uniform emission reduction strategies were compared to realistic control strategies (e.g, RACT, FMVECP), the difference in effectiveness of lowering peak ozone levels do not appear to be substantial.

Implication: Temporal, spatial, and reactivity effects of control strategies do not appear to substantially affect the regional ozone peak. However, spatial and temporal patterns of ozone throughout the region were not evaluated, so other differences between uniform reductions and realistic control strategies may be found.

1.0 INTRODUCTION

Detailed Photochemical Air Quality Simulation Models (PAQSMs) have been identified as having the greatest potential for estimating the effectiveness of control programs designed to reduce ambient levels of ozone.[1] Compared to other simpler models, the complex PAQSMs contain more detailed mathematical respresentations of the chemical and physical phenomena leading to ozone formation in the atmosphere. However, the complex nature of these models generally require considerable amounts of input data and their operation is often costly. These factors will likely preclude their use in many instances, necessitating the use of simpler models in their place. Because PAQSMs are generally perceived as providing the best estimate of the relationship between ozone and its precursors, the limited number of cases in which they have been applied can serve as one basis for evaluating the performance of simpler models. In this study, control program effectiveness predictions of two simple models - the City-specific Empirical Kinetic Modeling Approach (EKMA) and Proportional Rollback - are compared to those obtained with a more complex PAQSM.

Testing the performance of the simpler models by comparing their predictions to those of the PAQSM as a measure of model validity has two major shortcomings. First, when a PAQSM is applied to simulate existing (or base case) conditions, the PAQSM model predictions may not always agree precisely with observations. Such discrepancies could be due to errors in model inputs, observational errors, or in the mathematical representations of the ozone forming phenomena. More importantly, however, no guarantee exists that the more complex PAQSMs will accurately simulate changes from base conditions, such as reduced precursor emissions. A complete validation, as implied by this last limitation, cannot be conducted until emission reductions are actually imposed and the observed effects are compared with the PAQSM predictions. Unfortunately, the data base necessary for such complete model validation does not exist. While the second shortcoming cannot be circumvented, the first can be alleviated to some degree by selecting for evaluation only those PAQSM results corresponding to cases in which model predictions and observations agree reasonably well in the base case. Even though no absolute validation is possible, the possibility of

errors in the input data should be minimized because of the agreement between PAQSM predictions and observations in the base case. As a result, greater confidence is usually placed in the PAQSM predictions of control program effectiveness for those days when the PASM simulates base case observations accurately.

As indicated above, the primary focus of this study has been to compare the predictions of control program effectiveness of two simple models with those of a more complex PAQSM. The remainder of this chapter provides background information on the model applications and defines terms referred to throughout the text. The succeeding chapters describe the details of the model applications, the results of the model comparisons, and the conclusions and recommendations arising from those comparisons.

1.1 Background

An indepth study has been undertaken by the U.S. Environmental Protection Agency (EPA) to evaluate the performance of PAQSMs.[2] One phase of that study consists of applying a photochemical dispersion model developed by Systems Applications, Incorporated - the Urban Airshed Model. In this application, the detailed St. Louis Regional Air Pollution Study (RAPS) data base is used to derive the inputs necessary to carry out model simulations. A number of days have been simulated to evaluate the Airshed Model's performance in characterizing ozone formation under conditions relevant to the data collection period (1975 and 1976). In addition, a series of detailed sensitivity tests have been conducted for three of these days in order to:

(1) identify those model inputs which most significantly affect model predictions and subsequently require most care in data collection efforts;

(2) isolate possible sources of error in model inputs or formulation;

(3) estimate the effects of changes in precursor emission levels on predicted ambient ozone levels.

The results of this last set of sensitivity tests provide the basis for evaluating the two simpler models. Thus, the principal question addressed in this study is whether or not the effects of emission changes predicted by the simpler models are comparable to those predicted by the more complex Airshed Model.

The preceding question would, at first, seem straightforward. However, the manner in which these models are applied and the information provided by each complicates the problem to some extent. For example, the Airshed Model predicts pollutant concentrations, resolved both temporally and spatially throughout the modeling region. The regional peak ozone concentration predicted by the Airshed Model may not agree with the observed peak simply because an ozone monitor was not positioned near the location of the predicted peak. The implications of such a disagreement with regard to regulatory applications have not been fully resolved. Also, the Airshed Model prediction at the site of the observed peak may be higher or lower than the measured level. Like the aforementioned problem, procedures for incorporating these potential discrepancies in a regulatory application have not been determined to date. On the other hand, City-specific EKMA is by definition an empirical approach, depending on measured levels of ozone. The effects of proposed changes in precursor emissions (i.e., hydrocarbons and NO_x) are evaluated relative to the initial measured ozone level. The proportional rollback model is essentially also an empirical type model. As with City-specific EKMA, the base, or starting, point is determined by the measured ozone maximum. Thus, the distinct possibility exists that the simple models and the complex PAQSM could have significantly different base case conditions in terms of peak ozone, since the simple models rely solely on observations while the PAQSM has the capabilities of predicting ozone at locations for which monitoring data are unavailable.

To circumvent this problem, two separate procedures were followed in comparing the various models. The first entails using the Airshed Model prediction of peak ozone as the base case, despite any discrepancies between predicted and observed ozone peaks. On the other hand, the simple models are used exactly as they would be applied in practice, relying entirely on the

measured peak. The basis for comparison with these tests is the relative change in ozone maxima from the base case. For example, if an Airshed Model simulation was conducted in which hydrocarbon emissions were reduced by 50%, the percent change in the predicted regional peaks is computed, and that relative change is compared to the relative changes in peak ozone predicted by the other models. To some degree, this puts the model predictions on a common basis, even though they are starting from different bases. The second approach consists of developing the inputs for the simple models on the basis of Airshed Model simulations (i.e., the Airshed Model peak ozone would be used as input to the City-specific EKMA and Proportional Rollback models). For example, if the Airshed Model predicted a peak ozone level of 0.30 ppm, this value would be used as the base, or starting, point for the siample models, regardless of the observed peak ozone value. In effect, this procedure involves "modeling a model," and also puts the model predictions on a common basis.

Of the two procedures described in the preceding paragraph, the first is the most rigorous test of the simple models' performance. For those cases in which either of the simple models would be applied, the detailed data base required for the Airshed Model would not normally be available, nor would the PAQSM predictions. Thus, the results of the simple models would have to be relied upon entirely. However, the second set of tests may help to explain potential discrepancies between models. For example, consider the situation in which the predicted Airshed Model peak is at a location with no nearby ozone monitor. The sensitivity of this peak level to changes in precursor emissions may be different from that associated with the measured peak. Thus, even though a simple model may not agree with the PAQSM in the rigorous test, agreement may exist if the conditions corresponding to the PAQSM predicted peak are evaluated. Of course, a major limitation of the simpler models is that they do not have the spatial and temporal predictive capabilities of the PAQSMs (i.e., they rely entirely on observations). This is a limitation that cannot be overcome.

One additional set of hypothetical tests was conducted. In the Airshed Model sensitivity tests, the effects of increased hydrocarbon emissions were

simulated. Because of the implementation of control programs, these tests would not appear to be relevant for evaluating models which will be used to establish emission reductions necessary to reduce peak ozone levels. However, they afford the opportunity to examine the performance of the simpler models under conditions which may be characteristic of cities with higher prevailing HC/NO_x ratios than the ratios observed during the St. Louis RAPS. The procedure followed for these tests was to select, as the base case, the Airshed Model simulation with the highest hydrocarbon emissions, i.e., a test in which hydrocarbon emissions were deliberately increased above existing levels. The two simpler models were then used to model the Airshed Model simulations, and the sensitivity of peak ozone to changes in precursor emissions was evaluated from this starting point rather than the observed, or true, base case. These tests may be particularly illuminating when comparing City-specific EKMA with Proportional Rollback. The higher emissions result in an increased HC/NO_x ratio, and afford an opportunity to compare the two simple models at that higher ratio. The results of the tests have implications for the use of these two models in areas which exhibit HC/NO_x ratios which are higher than those found in the St. Louis area.

In viewing the model applications that follow, it must be emphasized that this study is not intended to determine the emission reductions necessary for the St. Louis area to achieve the ozone standard. Rather, it is intended to compare three air quality models. It should be remembered that the RAPS data base covers the 1975-1976 time period. A regulatory analysis for St. Louis will require an updated data base.

1.2 Definition of Terms

Throughout the text, frequent reference is made to a number of specialized terms and acronyms. For reference, several are defined below.

Hydrocarbons - This term is somewhat of a misnomer, but is used throughout the report for simplicity. It refers to emissions of Volatile Organic Compounds (VOC) except methane. Ambient concentrations of hydrocarbons refer to ambient levels of Nonmethane Organic Compounds (NMOC).

NO_x - Nitrogen oxides refer to the sum of Nitric Oxide (NO) and Nitrogen Dioxide (NO_2).

O_3 - Ozone

RACT - This acronym is used to represent the Application of Reasonably Available Control Technology to stationary sources of hydrocarbon emissions.

FMVECP - This acronym represents the implementation of the Federal Motor Vehicle Emission Control Program to reduce emissions of vehicular sources.

PAQSM - Photochemical Air Quality Simulation Models refer to the most detailed air quality models used to simulate ozone formation in urban areas.

City-specific EKMA - The term refers to a simple trajectory model used according to the guidelines outlined in Reference 10.

Rollback - Rollback is a simple air quality model in which the nonbackground portion of ozone is assumed to change equally proportional with changes in hydrocarbon emissions.

2.0 AIRSHED MODEL SIMULATIONS

The Airshed Model is a complex PAQSM of the Eulerian (or grid) type.[3] A network of grid cells is overlaid on the region to be modeled and the physical and chemical phenomena leading to ozone formation are mathematically simulated. These processes include emissions of primary pollutants (i.e., hydrocarbons and NO_x) into each cell, the advection of pollutants from cell-to-cell, chemical transformations of pollutants into intermediate and secondary species, transport of pollutants into the modeling region from upwind areas, and entrainment of pollutants from aloft due to growth in the mixed layer. The model computes pollutant concentrations within each cell continuously and thus attempts to reproduce pollutant-concentration time profiles measured at each monitoring site within the modeling region.

In the St. Louis application,[2] the area modeled is 60 km wide in the East-West grid direction and 80 km in the North-South. The horizontal dimensions of each cell are 4 km x 4 km. Each 4x4 km area is divided into four individual cells in the vertical dimension: the bottom two cells making up the mixed layer, and the two upper cells corresponding to the region above the mixed layer. Pollutant concentrations initially within each cell are estimated from available ambient measurements. Hourly emissions of primary pollutants injected into each cell are input through the simulation period which begins at 0500 Central Standard Time (CST) and ends at 1700 CST. The chemical transformations are represented by a detailed chemical mechanism named Carbon Bond II, which describes the NMOC-NO_x-O_3 photochemical interactions. The concentrations of pollutants transported into the modeling region are determined from measurements taken at locations outside, and upwind, of the modeling region. Finally, cell-to-cell advection is fixed by a wind field analysis routine which resolves measured wind data into u (east-west) and v (north-south) components within each cell.

Figure 2-1 illustrates the horizontal grid structure relative to the St. Louis area and the monitoring network. Note that the modeling region encompasses 21 RAPS monitoring sites from which much of the modeling inputs are derived, as well as providing the air quality measurements necessary to evaluate the model's performance. (Continuous measurements of wind speed,

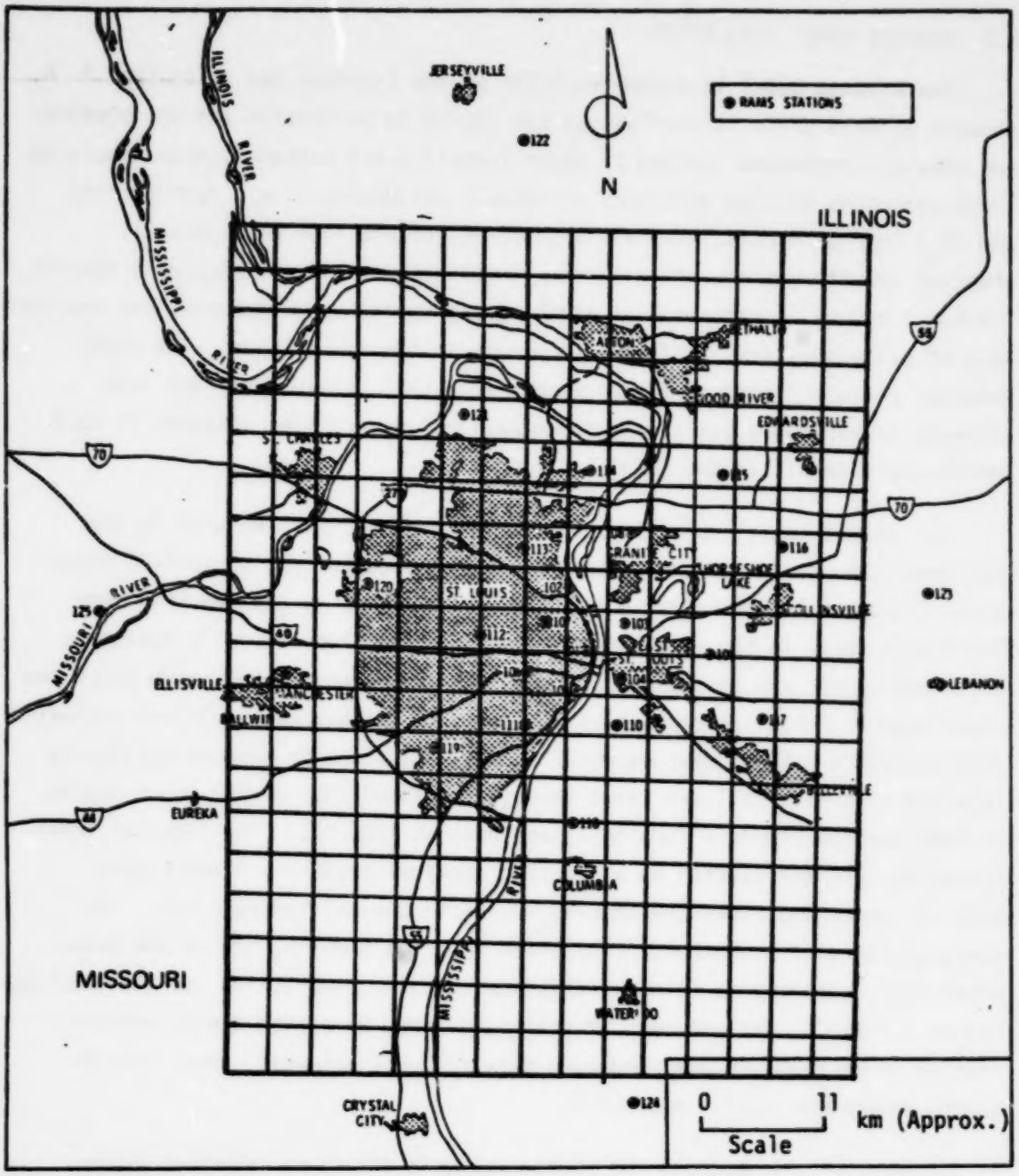

Figure 2-1. St. Louis Modeling Region.

wind direction, NMOC, NO, NO_2, and ozone, among others, were taken at each site.) The outer four sites (i.e., Sites 122-125) are used to determine the boundary concentrations which set pollutant transport into the modeling region. For a more detailed discussion of the Airshed Model application, the reader is referred to Reference 2.

2.1 Base Case Simulations

This section describes the results of applying the Airshed Model to simulate ozone formation on three days in the St. Louis region. Recall from Chapter 1 that the Airshed Model should reproduce observed ozone concentrations reasonably well to serve as the basis for evaluating the performance of simpler models. While a detailed evaluation of the Airshed Model's performance in the base case simulations is beyond the scope of this study, some rudimentary analysis can provide insight into overall model performance.

The three selected days are June 7, 1976 (Julian Day 159), July 13, 1976 (Day 195) and October 1, 1976 (Day 275). Each of these days is characterized by different meteorological regimes, thus serving to provide a broad basis for model evaluation and for investigating the effectiveness of control programs. Day 159 is one of moderate transport characterized by a persistent, light southeasterly flow. The peak one-hour average ozone concentration was 198 parts per billion (ppb), measured at Site 122, located well to the north of the central urban area. Early morning concentrations of NMOC and NO_x within the urban core were relatively high, and the estimated ozone concentration above the early morning mixed layer was the highest of the three days. On Day 195, winds were light to moderate out of the southeast. The measured NMOC and NO_x concentrations in the urban core on this day were much lower than those of the other two days, while a moderate level of ozone aloft was estimated. Nevertheless, the measured one-hour average peak ozone was the second highest of the three days - 223 ppb at Site 114 slightly north of the urban core. Day 275 had the highest measured ozone concentration of the three days - 244 ppb at Site 102 in the northern portion of the urban core. This day was marked by extreme stagnation with high early morning precursor levels in the urban core. The estimated level of ozone aloft was the lowest of the three days. Some of the key measurements and Airshed Model inputs characterizing the three days are summarized in Table 2-1.

Table 2-1. Summary of Miscellaneous Measurements and Airshed Model Inputs.

	Julian Day		
	159	195	275
Measured O_3 peak, ppb	198	223	244
Site of measured O_3 peak	122	114	102
Time of observed peak, CDT*	1600-1700	1600-1700	1500-1600
Measured 6-9 a.m. CDT urban average** NMOC, ppmC	1.8	0.2	1.9
Measured 6-9 a.m. CDT urban average** NO_x, ppm	.205	.048	.236
Measured 6-9 a.m. CDT urban average NMOC/NO_x ratio	7.6:1	7.0:1	8.1:1
O_3 level aloft input to Airshed Model, ppb	114	78	63
0800-1500 CDT network average wind speed, m/sec***	1.0	2.3	0.6
Maximum afternoon mixing height input to Airshed Model, meters	1972	1853	529

* CDT, Central Daylight Time

** Urban averages computed from the 6-7, 7-8 and 8-9 a.m. average measured at Sites 101, 102, 104, 105, 106, and 107. The reported NMOC/NO_x ratios are the averages of the six site-ratios, and thus do not necessarily equal the ratio of the urban average concentrations.

*** From Reference 3

Of principal interest (although not necessarily the best indicator of model performance) is the Airshed Model's prediction of regional peak ozone concentration. Figure 2-2 was constructed to compare the model's predictions with observations in terms of magnitude, location, and timing of the ozone peaks. In this figure, the large rectangle indicates the modeling region while the smaller one shows the relative location of the urban core. The location of the Airshed's prediction of peak ozone is denoted by a "□" while the location of the observed peak is marked by an "O". The magnitude and time of the corresponding peaks are shown to the right of each diagram, along with the percent difference between observed and predicted peaks. The figure clearly indicates significant differences between predicted and observed peaks in terms of magnitude and location. However, these differences are not necessarily indicative of model accuracy. For example, the Airshed regional peak on Day 159 is at a location with no nearby monitor, while the actual observed peak was outside the modeling region. On the other hand, the predicted regional peak for Day 195 is somewhat lower than the observed peak indicating a model underprediction. For Day 275, the magnitude of the peaks is similar, although the locations are somwhat different.

To provide a better indication of overall model performance, the Airshed Model predictions of ozone at each of the 21 monitoring locations within the modeling region were compared to the measured levels.* The most rigorous test involves comparing the observed ozone peak at each site with the ozone level predicted by the Airshed Model precisely at the time of the observed peak. The results of this test are illustrated graphically in the left-hand portion of Figure 2-3. When the timing criterion is relaxed, the Airshed peaks predicted at each monitoring site are compared to the observations, regardless of the time of the peak. These results are shown in the right hand portion of the same figure. In each of the individual graphs in Figure 2-3, the predicted

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* Actually, the Airshed Model predicts cell-wide average concentrations, not point concentrations necessary for direct comparison with monitored pollutant concentrations. In the discussions that follow, the average concentrations in the ground level cell corresponding to each monitor are compared to the measured levels.

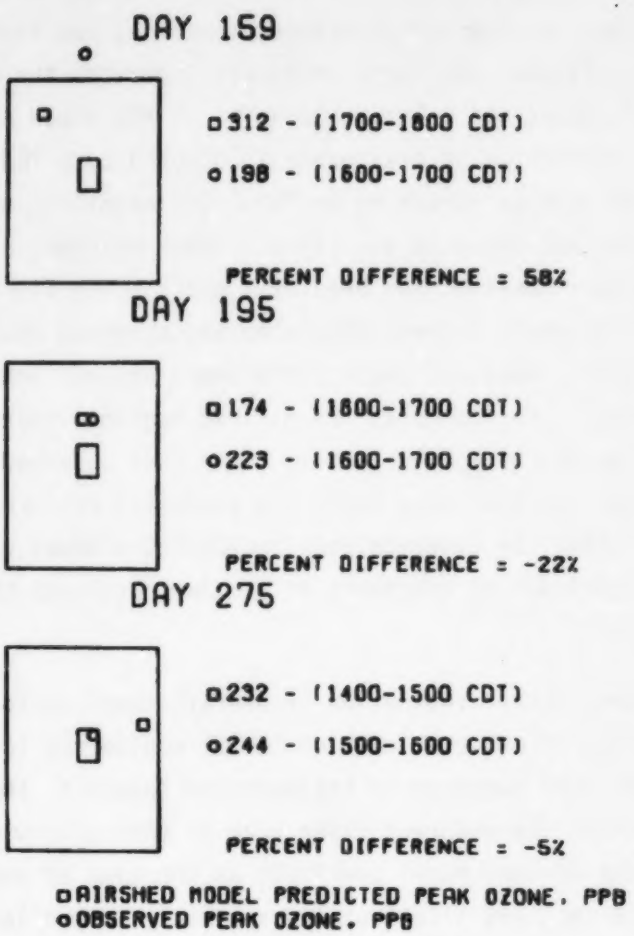

Figure 2-2. Airshed Predicted and Observed Regional Peak Ozone.

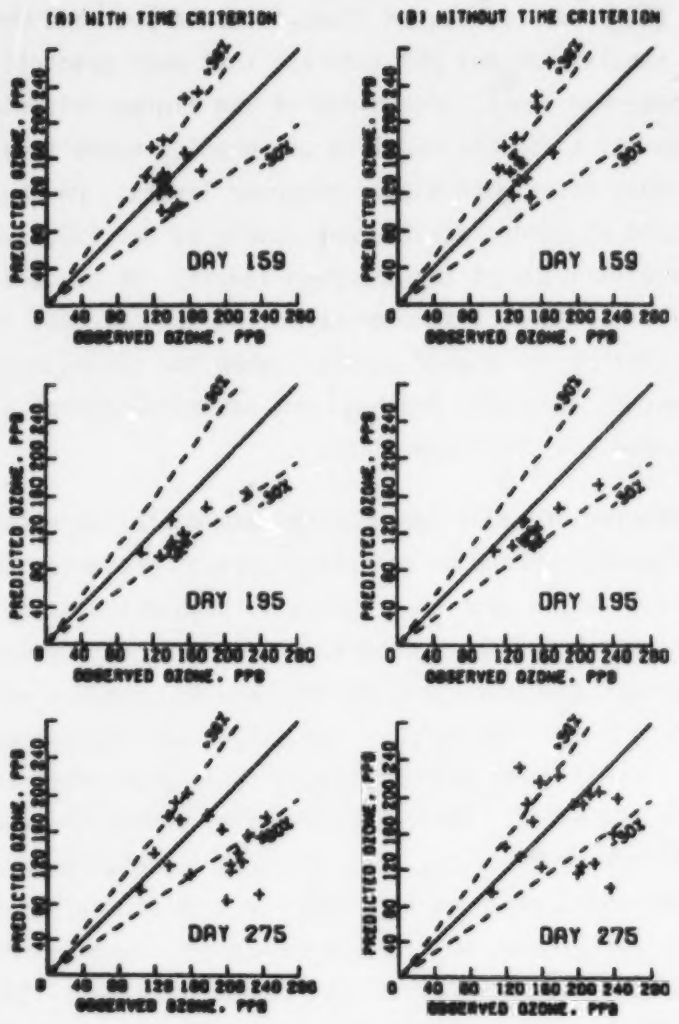

Figure 2-3. Airshed Predictions Versus Observations of Peak Ozone.

ozone (y-axis) is plotted versus observed ozone (x-axis). For reference, the 45 degree line (solid) indicates perfect agreement between predictions and observations, while the other two dashed lines indicate over-and under predictions of ±30%. The results for Day 159 indicate that most predictions are within ±30% of the observed level, regardless of the timing criterion. However, a tendency does exist for the model to overpredict ozone levels on this day, especially at those sites with higher measured levels. On the other hand, the Airshed Model tends to underpredict ozone levels on Day 195, even though most predictions are within 30% of the observed levels. On Day 275, the most rigorous test indicates a tendency to overpredict at the observed low ozone levels, and underpredict at the higher levels. When the timing criterion is relaxed, the agreement is improved somewhat, but underpredictions at locations with high measured ozone are still prevelant.

A detailed evaluation of model performance should, to the extent possible, address how well the model reproduces concentrations of precursor patterns as well as ozone patterns. While such an analysis is beyond the scope of this study, particular attention was focused on the Airshed Model's predictions of early-morning, urban core concentrations of NMOC and NO_x because of the implications for applying City-specific EKMA. (The latter will become evident in the next chapter.) Airshed Model predictions of these precursors are compared to observed levels in Table 2-2. General patterns of precursor levels were reproduced by the Airshed Model (e.g., high precursor levels on Days 159 and 275, low levels on Day 195), although a tendency for underprediction was found. (Note that in every case, NO_x is underpredicted, ranging from 14% to 42%, while on two of the days NMOC levels were underestimated.) The urban core, 6-9 a.m. NMOC/NO_x ratios predicted by the Airshed Model agree reasonably well with the ratios derived from ambient measurements.

The elementary analyses just described were not intended to assess conclusively the accuracy of the model, nor do they provide a complete picture of model performance. However, they do give some insight into how well the model is reproducing observed ozone levels. In most instances, predicted ozone levels at the locations of monitoring sites are within ±30% of the observations. Except for Day 159, the model tends to underpredict the higher ozone levels.

Table 2-2. 6-9 a.m. Urban Core Precursor Predictions Versus Observations*

	Predicted	Observed
Day 159		
6-9 a.m. CDT urban average NMOC, ppm	1.2	1.8
6-9 a.m. CDT urban average NO_x, ppm	.152	.205
6-9 a.m. CDT urban average NMOC/NO_x	8.1:1	7.6:1
Day 195		
6-9 a.m. CDT urban average NMOC, ppm	0.2	0.2
6-9 a.m. CDT urban average NO_x, ppm	.028	.048
6-9 a.m. CDT urban average NMOC/NO_x	8.9:1	7.0:1
Day 275		
6-9 a.m. CDT urban average NMOC, ppm	1.5	1.9
6-9 a.m. CDT urban average NO_x, ppm	.203	.236
6-9 a.m. CDT urban average NMOC/NO_x	7.7:1	8.1:1

* Urban average NMOC and NO_x levels are computed from the 6-7, 7-8, and 8-9 a.m. averages at Sites 101, 102, 104, 105, 106, and 107 and the cells corresponding to those sites. The NMOC/NO_x ratios are the average of 6-9 a.m. ratios at the individual sites (cells), thus, they do not necessarily equal the ratio of the urban average concentrations.

On Day 159, the model is biased towards overprediction at most monitoring sites. Finally, a tendency exists for the model to underpredict the early-morning precursor levels within the urban core.

2.2 Reductions in Hydrocarbon Emissions

A number of sensitivity tests were conducted to assess how the Airshed Model predictions of ozone respond to changes in hydrocarbons. These tests were designed primarily to indicate the potential effectiveness of hydrocarbon emission reduction programs. To establish this sensitivity over a wide range, reductions of 17%, 42% and 75% (from base levels) were tested. These reductions were applied uniformly to area and point source hydrocarbon emissions, as well as to initial NMOC concentrations.* Boundary conditions were held constant in all simulations.

Figure 2-4 summarizes the sensitivity results with respect to changes in the predicted peak ozone levels. The large boxes represent the modeling region, with the inner ones indicating the urban core. One diagram is included for each simulation. On each, the location, time and magnitude of the predicted peak ozone are shown. The first apparent result is that ozone levels are lowered by reductions in hydrocarbons, although the relative changes are different. For example, a 75% reduction in hydrocarbons gives ozone reductions between 41 and 64%, depending on the particular day. Secondly, the results indicate that, as hydrocarbons are reduced, the peak ozone level is likely to occur slightly farther from the city (i.e., farther downwind). Although not universally true, the peak often occurs later in the day under an emission reduction scenario.

Figure 2-5 illustrates the simulation results in another way. First, regional peak ozone concentrations are graphed against hydrocarbon reductions, followed by a graph showing the relative change (i.e, percent change) in ozone

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* Clearly, a realistic control program would not produce uniform emission reductions. However, the uniformity assumption makes the task manageable and eliminates the need to make some arbitrary assumptions regarding point versus area reductions. More realistic control strategies are discussed in Section 2.4.

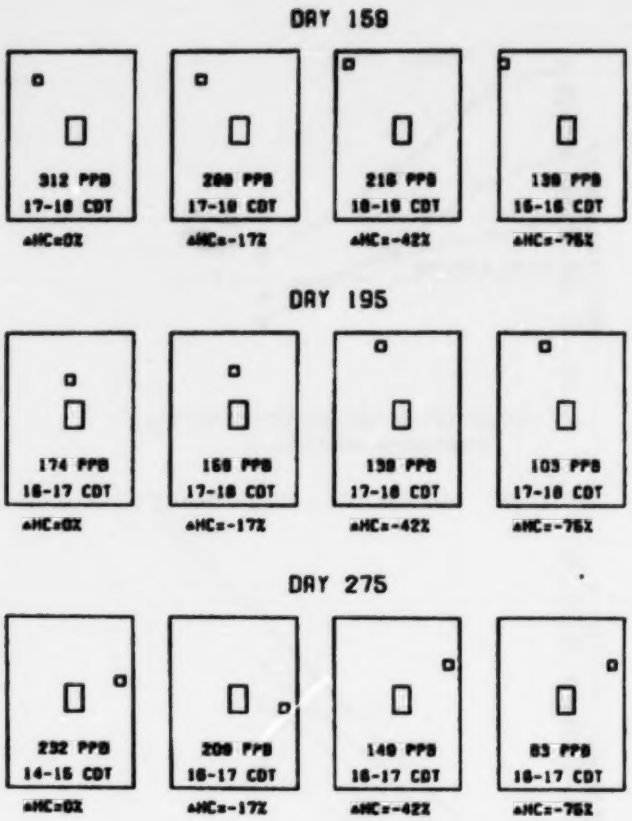

Figure 2-4. Summary of Airshed Model Simulations.

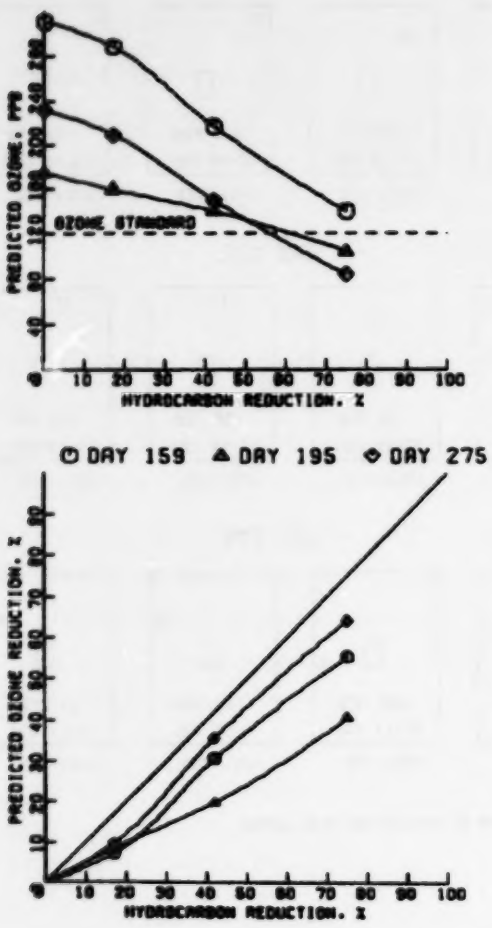

Figure 2-5. Airshed Model Sensitivity of Regional Peak Ozone to Hydrocarbon Reductions.

accompanying the hydrocarbon reductions. In this last figure, a line of unit slope is included as reference to indicate equally proportional changes between hydrocarbons and ozone. The figures clearly indicate that the O_3 response to changes in hydrocarbon is different for each day. The Airshed Model predicts the largest incremental changes in O_3 on Day 275, while Day 195 exhibits the least response. In every case, the percent change in ozone predicted by the model is less than the percent change in hydrocarbons input to the model. These findings are not entirely surprising since boundary conditions remained unchanged in all simulations, and one might expect the importance of boundary conditions to vary from day to day.

In examining Figure 2-5, one may be tempted to estimate the emission reduction necessary to achieve the National Ambient Air Quality Standard (NAAQS) for ozone. Several caveats are in order. Recall that in the base case simulations, the Airshed Model predictions of regional peak ozone did not agree precisely with measured peaks. In fact, a large difference existed on Day 159. Whether or not the Airshed Model's predicted peak would be accepted as the basis for a regulatory application has not been resolved. Secondly, as described above, boundary conditions were not changed in any simulation. In a regulatory application, some estimate of future boundary conditions might be factored into the model applications (e.g., the level of ozone aloft might be altered to reflect the implementation of upwind control programs in the future).[1] Finally, the modeling results provide information on how the O_3 levels change on any particular day. To establish the control needed to meet the ozone standard, this information must be related to the statistical form of standard. The latter allows, on average, one maximum daily value to be greater than 0.12 ppm at each site during a year.[4] Procedures for relating the model output to the form of the standard are being explored, but have not yet been prescribed. Thus, the information presented in Figure 2-5 could not necessarily be used to estimate reduction in hydrocarbon emissions needed to achieve the ambient ozone standard.

2.3 Reductions in Hydrocarbons in an Area With a High HC/NO_x Ratio

Previous studies have suggested that the $NMOC/NO_x$ ratio is an important factor in ozone formation potential.[5,6,7] In the base case simulations previously described, observed early-morning urban core $NMOC/NO_x$ ratios were about 8:1, while the molar ratio of hydrocarbon emissions to NO_x emissions is on the order of 6:1. Evidence exists to suggest that higher $NMOC/NO_x$ ratios may be prevalent in some urban areas.[8] Consequently, a sensitivity analysis was formulated to evaluate the effectiveness of hydrocarbon emission reductions starting from a base point with higher $NMOC/NO_x$ ratios. For each day, an Airshed Model simulation was conducted in which hydrocarbon emissions and initial concentrations were increased by 67%, giving an emission ratio of 10:1 and ambient ratios around 13:1. These simulations were in turn used as base cases, and the previously described simulations were evaluated as if they reflected reductions from this new, hypothetical base case.

The simulation results are summarized in Figure 2-6. Most findings are comparable to results of the previous section (see Figure 2-4). As hydrocarbons are reduced, ozone is reduced, although the reductions in ozone are less than the hydrocarbon reductions input to the model. Peak ozone levels predicted by the model tend to occur farther downwind and later in the day, commensurate with higher reductions. Differences in responses of peak ozone levels to changes in hydrocarbon emission reductions under the high HC/NO_x ratio scenario versus the lower ratio conditions are highlighted in Figure 2-7. Clearly, the model response on two days is quite similar, while that on Day 159 is markedly different. In the latter case, the higher ratios imply that a greater hydrocarbon reduction is required to achieve a comparable relative change in ozone levels. Stated another way, the model is less sensitive to changes in hydrocarbons than in the lower ratio case. Obviously, this is not true for Days 195 and 275.

2.4 Control Strategy Predictions

The emission changes described in the previous two sections were hypothetical in nature, i.e., changes were made uniformly throughout time and space. While providing useful information, they are not truly indicative of realistic control

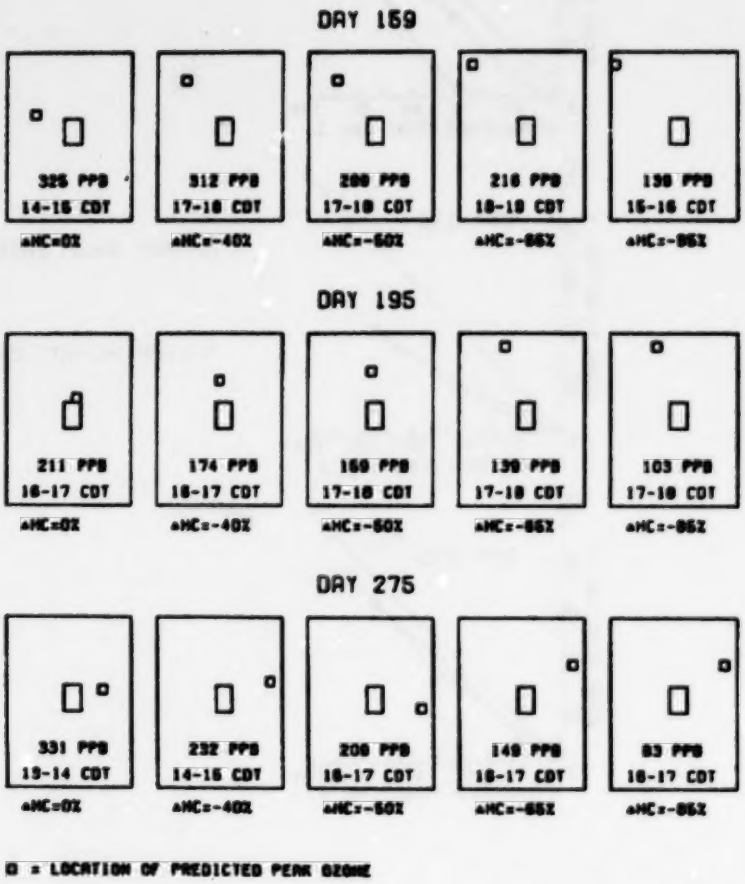

Figure 2-6. Summary of Airshed Simulations for the High HC/NO_x Case.

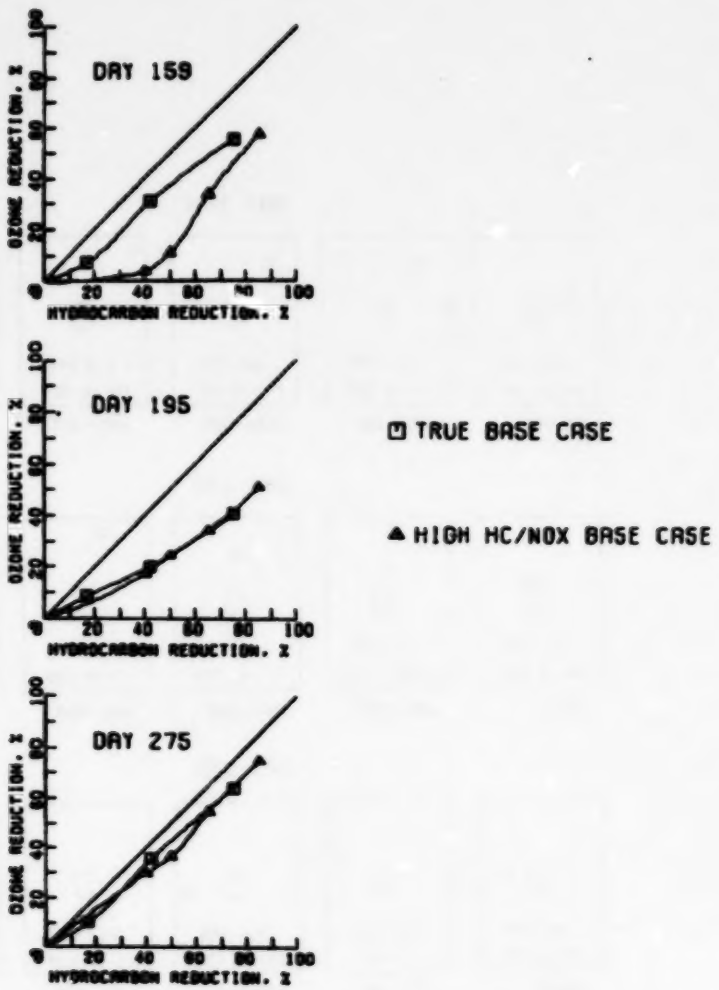

Figure 2-7. Comparison of Sensitivity to Hydrocarbon Reductions.

strategies, which inherently contain spatial and temporal nonuniformities. A series of three strategies have been simulated for each day to assess the effectiveness of typical control strategies.[9] The first strategy consists of applying Reasonably Available Control Technology (RACT) to stationary sources of hydrocarbon emissions identified in EPA's Control Techniques Guidelines.[16] A second control strategy was designed to simulate the effects of the Federal Motor Vehicle Emission Control Program (FMVECP). In this strategy, the hydrocarbon emissions from mobile sources alone were reduced to levels anticipated in 1987, as a result of vehicular control. Note that in the FMVECP strategy, only hydrocarbon emissions were changed (i.e., NO_x remained fixed). Finally, a combined RACT and FMVECP strategy was simulated.

Figure 2-8 contrasts the effectiveness of the control strategies in reducing regional peak ozone levels with the results of the uniform reduction scenario. Overall regional reductions in hydrocarbon emissions for the RACT, FMVECP and combined strategies were 22%, 34% and 56%, respectively. Note, however, that these reductions affect the spatial and temporal distribution of emissions, as well as the reactive mix of emissions. For example, the FMVECP strategy affects mobile source emissions only, and these emissions vary throughout the day. Furthermore, in the FMVECP strategy, some of the more reactive species are estimated to be removed to a greater extent than some of the less reactive constituents.* Thus, one may not expect the realistic control strategy to agree with a uniform emission reduction simulation in which hydrocarbons were reduced by a comparable amount. Somewhat surprisingly, however, the realistic control strategies tend to fall in line with the uniform reduction scenarios in most instances. Some shifting in the location and timing of the

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* The Carbon Bond II Mechanism contains five classes of reactive hydrocarbons - Paraffins, Ethylene, Olefins, Aromatics, and Carbonyls. The estimated effects of the FMVECP give larger reductions in Ethylene and Olefins than for any of the other constituents. Furthermore, it should be noted that some approximations were made in determining changes in area source emissions resulting from application of RACT and FMVECP. While these approximations may tend to smear the spatial and temporal effects somewhat, they would almost certainly be made in any application of the Airshed Model.

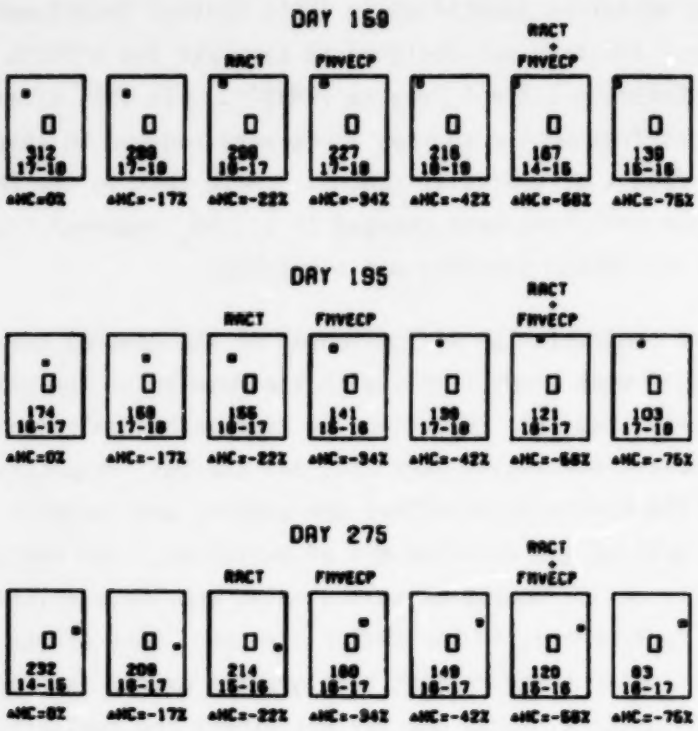

Figure 2-8. Summary of Airshed Control Strategy Simulations.

peaks is noted, but these differences are usually small. (Note, however, this conclusion may not apply to the temporal and spatial distribution of ozone levels throught the region.) To examine how changes in the magnitude of the peak compare to the uniform reduction scenarios, Figure 2-9 was prepared. In these graphs, the Airshed Model sensitivies to uniform changes in hydrocarbons (described in Section 2.3) are reproduced. Super-imposed on these graphs are the RACT, FMVECP and combined strategy results (note that the three points are not connected because they represent unique and distinct points). Again, a line of unit slope is included as reference to show equally proportional reductions. Although some differences do exist, the points generally follow the same patterns as found with the uniform strategies. The results do suggest the FMVECP strategy is usually more effective than the RACT strategy when applied independently. This would suggest that control of area source emissions would be of most benefit in reducing peak ozone levels. However, the model indicated that control of point source emissions results in significant additional reductions in ozone when implemented in conjunction with mobile source control.

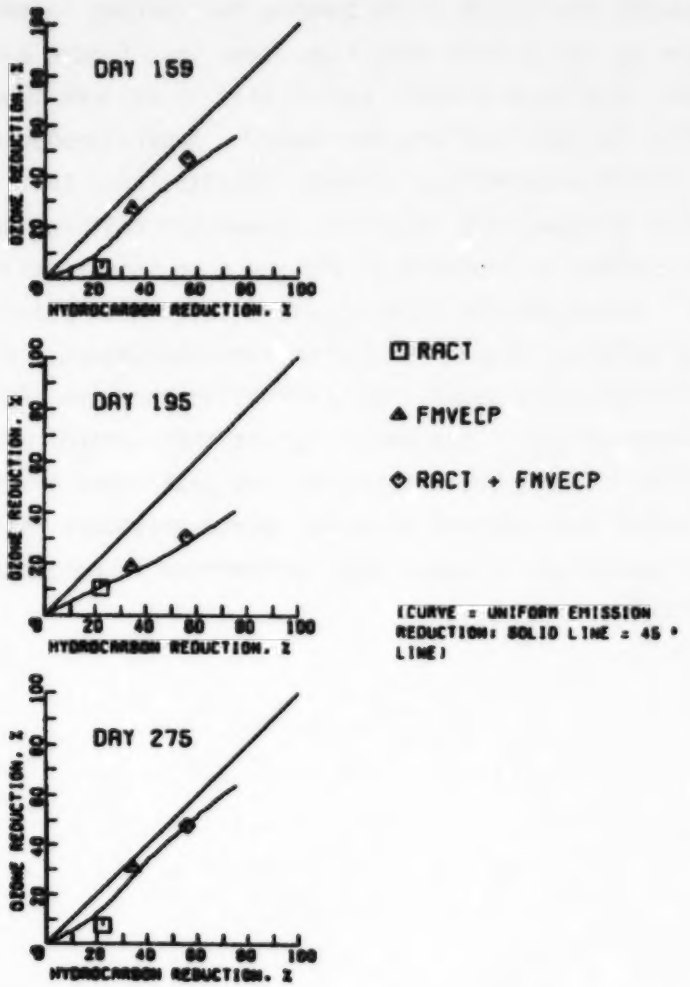

Figure 2-9. Control Strategy Effectiveness Compared to Uniform Emission Reductions.

3.0 EVALUATION OF SIMPLE MODELS

The Airshed Model results described in the previous section provide the ground work necessary for evaluating the two simpler models: City-specific EKMA and Proportional Rollback. The Airshed Model was used to predict how peak ozone levels respond to changes in hydrocarbons for a number of control scenarios. The question to be addressed now is whether or not the simple models predict similar effects. Before directly addressing this question, however, a brief discussion of the two simpler models is needed in order to clarify some of the comparisons to be made.

3.1 City-specific EKMA Applications

The City-specific EKMA technique has been described in numerous publications, but will be briefly discussed here for background.[1,10] This model uses a LaGrangian, or trajectory, concept. A well mixed column of air initially containing pollutants is envisioned to travel with the wind to the site of peak ozone concentration. As the column moves with the wind, emissions are injected into the column, the height of the column rises in accordance with the diurnal variation in mixing height (resulting in pollutant dilution within the column and entrainment of pollutants from aloft), and the HC-NO_x-O_3 photochemical interactions are simulated by means of a chemical mechanism.* By deriving the model inputs consistently with this concept, the model will simulate the formation of ozone within the column, and calculate the resultant peak one-hour average level occurring during the simulation period. Note that the trajectory model does not have the capability of reproducing overall spatial ozone patterns unless many trajectories are simulated separately.

The heart of the City-specific EKMA technique is the Ozone Isopleth Plotting Package (OZIPP)[11,12] computer model which incorporates, in mathematical form, the concepts described above. Inputs to the model can be divided into six categories: trajectory, sunlight intensity, dilution, pollutant

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* This chemical mechanism is <u>not</u> the same one incorporated in the Airshed Model.

transport, post-0800 emissions, and reactivity. Procedures for estimating the proper inputs have been described in Reference 10, and were used in this study. They are briefly summarized below:

1) Trajectory - the column of air originates in the center city and begins moving at 0800 CDT towards the site of peak ozone at a uniform speed;*

2) Sunlight Intensity - light intensity is calculated internally in the model from inputs on city location and simulation date;

3) Dilution - dilution is determined from mixing height measurements (early morning and maximum afternoon);

4) Pollutant Transport - level of ozone aloft was set to be the same as that used in the Airshed Model simulations;

5) Post 0800 Emissions - emissions derived from countywide emission inventories and the assumed trajectory;

6) Reactivity - all values recommended in Reference 10 were used (i.e., no changes in reactivity were evaluated with EKMA).

By estimating the above inputs and specifying the pollutant concentrations initially within the "column," the OZIPP model will compute the peak ozone concentration occurring in the column. This level can be compared to the peak measured at, or near, the end of the trajectory for a crude measure of the OZIPP model's capability to simulate accurately the ozone formation processes. For illustration, these absolute predictions have been made and three sets of comparisons performed. In the first, all OZIPP inputs are derived in accordance with the monitored peak on each day (i.e., the trajectory leads to the site of the measured peak) and the OZIPP prediction is compared to the observed peak. In the second set, all OZIPP inputs are derived according to Airshed Model predictions of peak concentration (i.e., the trajectory leads to the location

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* This assumption corresponds to that used in the Level III EKMA delineated in Reference 13.

of the Airshed Model's predicted peak) and the OZIPP predicted peak ozone is compared to the Airshed Model prediction. The last set of simulations is similar to the second, except that the hypothetical, high HC/NO_x, base case is used for comparison. In the last two sets of simulations, care was taken to replicate Airshed Model conditions as closely as possible in deriving OZIPP inputs. Thus, in effect, OZIPP is being used "to model a model."

Figure 3-1 illustrates the results. The top graph compares OZIPP predictions with observations on each of the three days. The bottom graph shows the OZIPP/Airshed Model comparisons. In all cases, the OZIPP predictions were within $\pm$30% of the observed levels or Airshed predictions, indicating relatively close agreement. However, it must be emphasized that this type of test is a very crude evaluation measure. For example, no assurance exists that the early-morning, urban core precursor cloud is directly responsible for the peak observation (i.e., the assumed trajectory may be incorrect). Thus, the possibility exists that the relatively good agreement is simply fortuitous.

While predictions of peak ozone can be made with OZIPP, the major function of the model is to generate ozone isopleth diagrams from which estimates of required controls are made, or from which the effectiveness of proposed control programs can be estimated. On such a diagram, peak concentrations of ozone are plotted in the form of isopleths versus initial NMOC and NO_x concentrations. These isopleths represent the model's predicted response of ozone peaks to changes in levels of hydrocarbons and NO_x. Because of the simplifying assumptions in the OZIPP model and the likelihood that the model predictions may not agree precisely with observations, the starting point on the diagram is established from <u>measured</u> O_3 and $NMOC/NO_x$ values (i.e., this has the effect of calibrating the model to existing conditions.) Control strategy effectiveness is then evaluated relative to the starting point on the diagram (e.g., changing HC X% and NO_x Y% will change ozone by Z%). In the City-specific EKMA applications discussed in the next few sections, the ozone peak and the $NMOC/NO_x$ ratio used to establish the starting point on the isopleth diagram are derived from ambient measurements or from Airshed Model output, as appropriate.

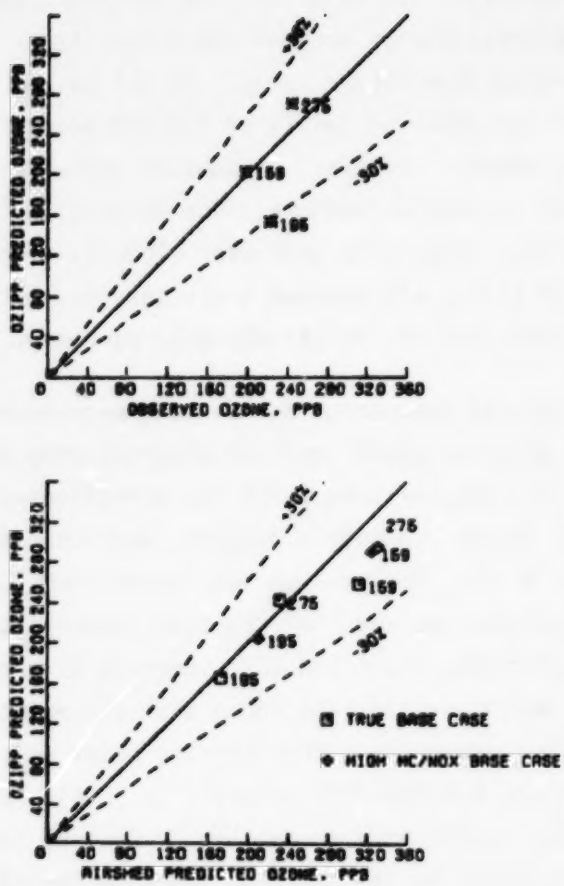

Figure 3-1. Comparison of OZIPP Predicted Ozone Versus Observed Levels and Airshed Model Predicted Levels.

3.2 Proportional Rollback Applications

The Proportional Rollback model is based on the concept that ozone concentrations change proportionally with hydrocarbon emissions. The model makes predictions in a relative sense in that changes in emissions are related to changes in air quality. Unlike OZIPP or the Airshed Model, Rollback cannot be used to make absolute predictions in a base case situation. The form of the Rollback Model considered here is:

$$\Delta HC = \frac{[(O_3)_E - B] - [(O_3)_F - B]}{(O_3)_E - B} \qquad (3\text{-}1)$$

where

ΔHC = fractional change in hydrocarbon emissions

$(O_3)_E$ = existing O_3 level

$(O_3)_F$ = future O_3 level

B = background O_3 level

In the calculations described below, background ozone was always assumed to be 1/2 of the base case level of ozone aloft on the particular day in question. Note that inclusion of a constant background ozone results in ozone changes which are less than changes in hydrocarbons (i.e., a 1:1 relationship does not exist). The factor of "1/2" was based on the work described in Reference 8. As with the City-specific EKMA applications, the existing ozone concentrations used correspond to either measured levels or Airshed Model peak predictions, as appropriate.

3.3 Reductions in Hydrocarbon Emissions

Section 2.2 described the results of the Airshed Model simulations in which hydrocarbons were reduced uniformly from base conditions. These simulations have been replicated, to the extent possible, with the two simple models. Two different sets of comparisons, along the lines described in Section 3.1, are made. The first involves comparing the models exactly as they would be applied, without trying to compensate for known model differences. For example, the base case ozone peaks used in City-specific EKMA and Proportional Rollback are measured levels, while base case peaks used with the Airshed Model are the

regional peaks predicted by Airshed. Other known differences in model inputs exist between Airshed and EKMA also (e.g., NMOC/NO_x ratio, dilution rate, etc.). This is a very severe test and provides information on the model predictions obtained under independent applications.

The second set of comparisons entails resolving known differences in model inputs to eliminate this as a potential source of discrepancy between models. In effect, the simple models were made to replicate, as closely as possible, the conditions in the Airshed Model. Another way of looking at this set of comparisons is that the simple models are being used to model the more complex Airshed Model. Such tests may provide some information regarding potential discrepancies found in the first set.

3.3.1 Independent Model Tests

Figure 3-2 shows the models' sensitivity to changes in hydrocarbons for each day. The first apparent result is that relationships between model responses differ according to the day being modeled. First, consider Day 159. Rollback and Airshed agree reasonably well, while City-specific EKMA is more conservative over most of the range of emission reductions (i.e., City-specific EKMA predicts a smaller reduction in ozone for a given hydrocarbon reduction). On Day 195, Airshed and City-specific EKMA agree reasonably well up to a 40% reduction in emissions. In this range, both models are substantially more conservative than rollback. At reductions greater than 40%, City-specific EKMA becomes substantially more sensitive than Airshed to incremental changes in hydrocarbons. On Day 275, Rollback and Airshed agree very well. While the agreement between Airshed and City-specific EKMA is reasonably good up to a hydrocarbon reduction of 40%. Again City-specific EKMA exhibits a greater sensitivity to HC changes at the higher reductions. These findings demonstrate that neither simple model reproduces the Airshed Model results over all conditions. For two days, Proportional Rollback is in closer overall agreement with the Airshed Model than is City-specific EKMA, but significant differences between Airshed and Rollback occur for one day (Day 195).

While the overall model responses are an important consideration, a major function of any of these models is to determine how much control is

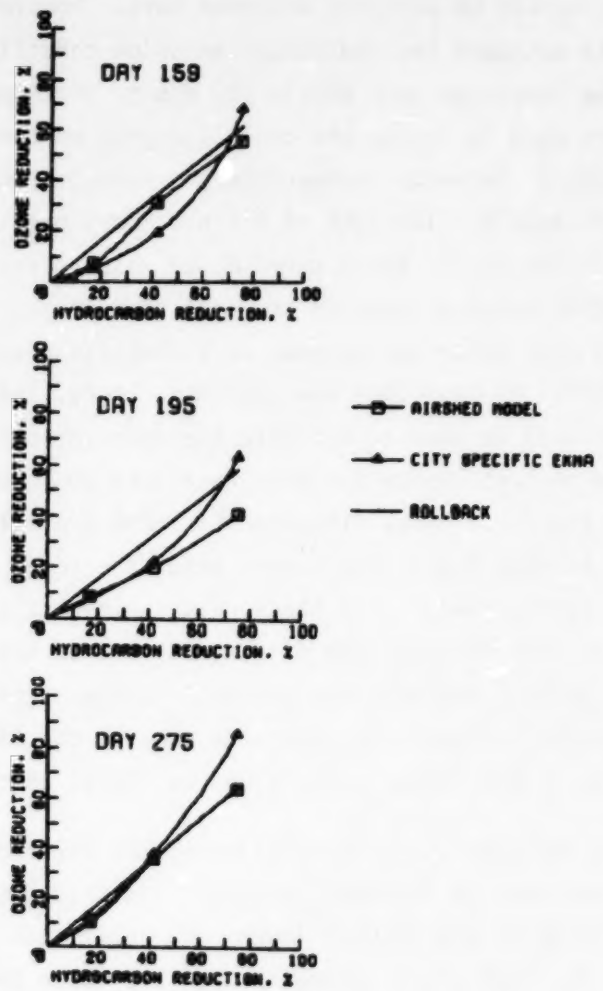

Figure 3-2. Comparison of Airshed, City-specific EKMA and Rollback to Changes in Hydrocarbons (Independent Tests).

needed to achieve the NAAQS for ozone. As briefly discussed in Chapter 2, this question cannot be directly answered here. However, each of the models can be used to estimate the individual emission reductions necessary to lower the peak ozone levels on each day to 120 ppb.* (Presumably, data such as these would be used in fixing the overall degree of control needed to achieve the ozone NAAQS.) Table 3-1 summarizes the results, assuming an independent application of models. Two sets of Airshed Model predictions are presented in the table. In the first, the Airshed Model results are used as is, regardless of discrepancies between observed and projected peaks. Shown in parenthesis is the second case which corresponds to a simplistic method for calibrating the Airshed Model to base case measurements. Here, the Airshed Model response curve (Figure 3-1) is used to estimate the hydrocarbon reduction that will give the same percent change in ozone necessary to lower the measured peak to 120 ppb. In the first case, City-specific EKMA predictions, when compared to those of the Airshed Model, are lower, about the same, and lower on Days 159, 195 and 275, respectively. For those days in which City-specific yielded lower controls than Airshed, the differences are on the order of 10%.** For this same situation, applying Proportional Rollback results in controls that are lower, about the same, and about the same as the Airshed Model. However, the difference in predicted controls on Day 159 is on the order of 20%.**

For the simplistic calibration of the Airshed Model to base conditions, the comparisons lead to different results. In this case, City-specific EKMA estimates of control are higher, lower, and lower than those of the Airshed Model, while Rollback gives estimates that are about the same, lower, and

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* It should be emphasized that in all calculations of hydrocarbon reductions, the boundary conditions were fixed at the base levels. In a true regulatory appion, some consideration may be given to altering boundary conditions to reflect the impact of upwind control programs. This is most important with respect to ozone aloft, especially with the simple models.

** On Day 159, the control needed to reduce the Airshed predicted peak of 120 ppb is outside the range of tests, and thus the difference could be somewhat greater.

Table 3-1. Emission Reductions Needed to Reduce Peak O_3 to 120 ppb.

Day		Airshed*	City-specific EKMA	Rollback
159	Base case peak O_3, ppb	312	198	198
	O_3 reduction necessary to lower peak to 120 ppb	62% (39%)	39%	39%
	HC reduction necessary to lower peak to 120 ppb	>75% (52%)	66%	56%
195	Base case peak O_3, ppb	174	223	223
	O_3 reduction necessary to lower peak to 120 ppb	31% (46%)	46%	46%
	HC reduction necessary to lower peak to 120 ppb	60% (>75%)	62%	56%
275	Base case peak O_3, ppb	232	244	244
	O_3 reduction necessary to lower peak to 120 ppb	48% (51%)	51%	51%
	HC reduction necessary to lower peak to 120 ppb	57% (59%)	47%	59%

* The HC reductions in parenthesis refer to the control needed to lower ozone by the same <u>percent</u> as the other two models.

about the same. Once again, when City-specific EKMA over or underpredicts the controls (as compared to Airshed), the differences are on the order of 10%. The single rollback prediction that differs from the Airshed Model estimate is lower by at least 20%.

The results just described are similar to the findings regarding the comparisons of overall model response, i.e., the comparisons yield mixed results. However, some important points should be made. When Rollback gave results that were different from Airshed, the estimated controls were lower by as much as 20% (i.e., the difference in controls was 20). On the other hand, differences between City-specific EKMA and the Airshed Model were usually on the order of ±10%. City-specific EKMA yielded significantly higher controls than Airshed in only one case (14% higher). Thus, based on these few comparisons, neither simple model would appear to consistently and significantly overestimate the hydrocarbon emission reduction necessary to lower peak ozone to the level of the standard.

3.3.2 Common Basis Tests

As described above, the comparisons of Section 3.3.1 were made on the basis of independent applications of the three models. In this section, comparisons of the models are made using the Airshed Model simulations as the basis, i.e., the simple models are made to replicate the Airshed base case situation as closely as possible. In this case, the Airshed Model predicted peaks are input to Rollback and City-specific EKMA. In addition, the NMOC/NO_x ratio input to City-specific EKMA was altered to agree with 6-9 a.m. ratio predicted by Airshed for the "urban core" (see Table 2-1). Additionally, the OZIPP program was modified to reflect more precisely the growth in mixing height embedded in the Airshed Model, and NMOC and NO_x concentrations aloft corresponding to Airshed Model inputs were input to City-specific EKMA.* Presumably, these modifications put the models on a more common basis and allow for more direct comparison of model results, mitigating possible discrepancies due to differences in model inputs.

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* The mixing height growth in Airshed is based on a piecewise linear fit to measured mixing heights. NMOC and NO_x levels aloft were on the order of .05 ppmC and .003 ppm, respectively.

Figure 3-3 depicts the relative changes in peak ozone as a function of changes in hydrocarbons. The results are not entirely different from those of the preceding section. However, the overall agreement between Airshed and City-specific EKMA is improved somewhat. Airshed and Rollback still agree fairly well on Days 159 and 275, although Rollback now exhibits greater sensitivity to changes in hydrocarbons at the lower emission reductions on Day 159. On this same day, City-specific EKMA's sensitivity is less than Airshed's, up to a control level of about 65%.

Table 3-2 summarizes the individual emission reductions predicted by each model which are necessary to lower the Airshed Model's peak ozone levels to 120 ppb. City-specific EKMA gives lower controls than Airshed in all three cases. The largest difference is 9%, although the possibility exists for a larger difference on Day 159. Rollback agrees fairly well with Airshed except for one case in which Rollback's control estimate was lower by 20% than Airshed (i.e., 40% versus 60%). Once again, neither simple model consistently overestimates controls needed to reduce peak ozone levels to 120 ppb.

These findings suggest that the model differences found in the previous sections are not entirely due to discrepancies in model input. Even when the models are put on a common basis, differences do occur. Neither simple model can reproduce the Airshed Model predictions over all conditions considered, but neither simple model consistently overestimates the hydrocarbon reductions necessary to reduce peak ozone levels to 120 ppb. While Rollback performs adequately in many cases, the potential for significant underprediction in some instances can be inferred. While City-specific EKMA does not always agree with the Airshed Model, substantial over- or underpredictions are not indicated with regard to the degree of control needed to lower peak ozone to the level of the standard.

3.4 Reductions in Hydrocarbons in an Area With a High HC/NO_x Ratio

Recall from Section 2.3 that a special set of simulations was conducted with the Airshed Model in which hydrocarbons were increased by 67%. These simulations were in turn used as hypothetical base cases to evaluate control program effectiveness at potentially high HC/NO_x conditions on each of the

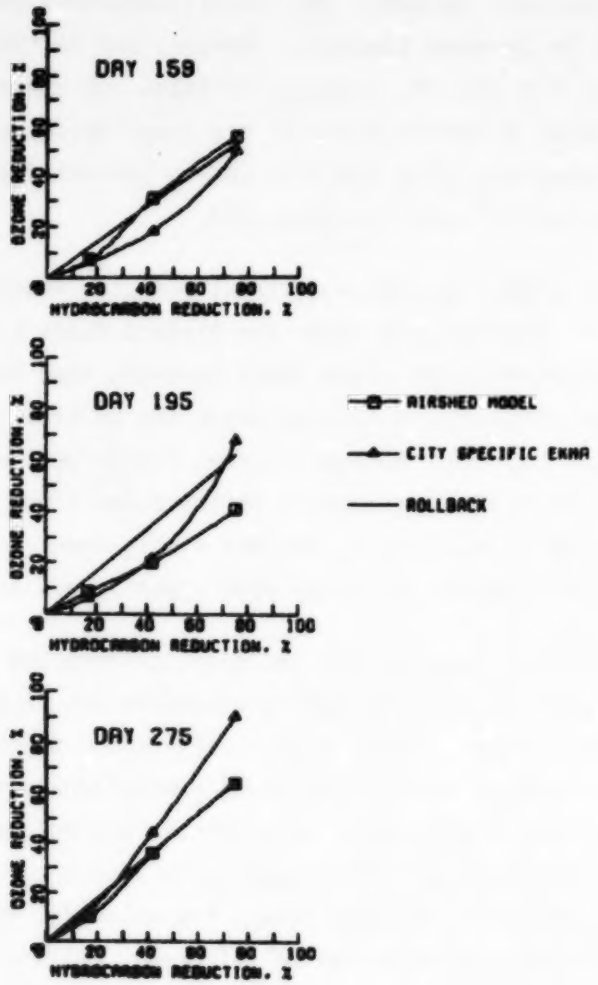

Figure 3-3. Comparison of Airshed, City-specific EKMA and Rollback to Changes in Hydrocarbons (Common Basis Tests).

Table 3-2. Emission Reductions Needed to Lower Peak O_3 to 120 ppb.

Day		Airshed	City-specific EKMA	Rollback
159	Base case peak O_3, ppb	312	312	312
	O_3 reduction necessary to lower peak to 120 ppb	62%	62%	62%
	HC reduction necessary to lower peak to 120 ppb	>75%	72%	75%
195	Base case peak O_3, ppb	174	174	174
	O_3 reduction necessary to lower peak to 120 ppb	31%	31%	31%
	HC reduction necessary to lower peak to 120 ppb	60%	51%	40%
275	Base case peak O_3, ppb	232	232	232
	Reduction in O_3 necessary to lower peak to 120 ppb	48%	48%	48%
	HC reduction necessary to lower peak to 120 ppb	57%	50%	56%

three days considered. These evaluations were reproduced with the simple models to investigate comparability under these conditions. (All simple model inputs were made comparable to the Airshed simulations.) Recall from the previous discussions that little difference in Airshed sensitivity was found except for Day 159. Figure 3-4 compares the Airshed Model sensitivity to those of the two simple models. Once again, neither of the simple models adequately reproduces the Airshed Model results in all cases. City-specific EKMA agrees fairly well on Day 159 but exhibits greater sensitivity on Day 195 and less on Day 275. Rollback's agreement with Airshed is relatively good on Day 275, but exhibits greater sensitivity on the other two days.

Table 3-3 presents the HC controls necessary to reduce each peak to 120 ppb. In this hypothetical scenario, City-specific EKMA and Airshed agree fairly well except for Day 195, in which the controls estimated with City-specific EKMA are lower by about 10% (i.e., 63% versus 75%). On the other hand, the estimates obtained with Rollback are all lower than those found with Airshed, with differences ranging from 5% to 22%. Consequently, under the high HC/NO_x ratio scenario, Rollback tends to give control requirements that are less than those of Airshed, while City-specific EKMA follows the Airshed results more closely.

3.5 Control Strategy Predictions

In Section 2.4, three realistic control strategies were simulated: the application of Reasonably Available Control Technology (RACT) to stationary sources; the effect of the Federal Motor Vehicle Emission Control Program (FMVECP); and the combination of the two. Regional emission reductions were about 22%, 34% and 56%, respectively. In this section, the predictions of strategy effectiveness obtained with the simple models are compared to those found with the Airshed Model. Recall that only Airshed has the capability of considering the spatial, temporal and reactivity effects found with these types of control programs. It is useful, however, to examine how the predictions of the simple models compare to those of Airshed for these more realistic control strategies. In the comparisons, two bases are again used: (1) the model applications are independent, and (2) the models are put on a common basis (i.e., inputs to all models are made comparable to the extent possible).

Table 3-2. Emission Reductions Needed to Lower Peak O_3 to 120 ppb.

Day		Airshed	City-specific EKMA	Rollback
159	Base case peak O_3, ppb	312	312	312
	O_3 reduction necessary to lower peak to 120 ppb	62%	62%	62%
	HC reduction necessary to lower peak to 120 ppb	>75%	72%	75%
195	Base case peak O_3, ppb	174	174	174
	O_3 reduction necessary to lower peak to 120 ppb	31%	31%	31%
	HC reduction necessary to lower peak to 120 ppb	60%	51%	40%
275	Base case peak O_3, ppb	232	232	232
	Reduction in O_3 necessary to lower peak to 120 ppb	48%	48%	48%
	HC reduction necessary to lower peak to 120 ppb	57%	50%	56%

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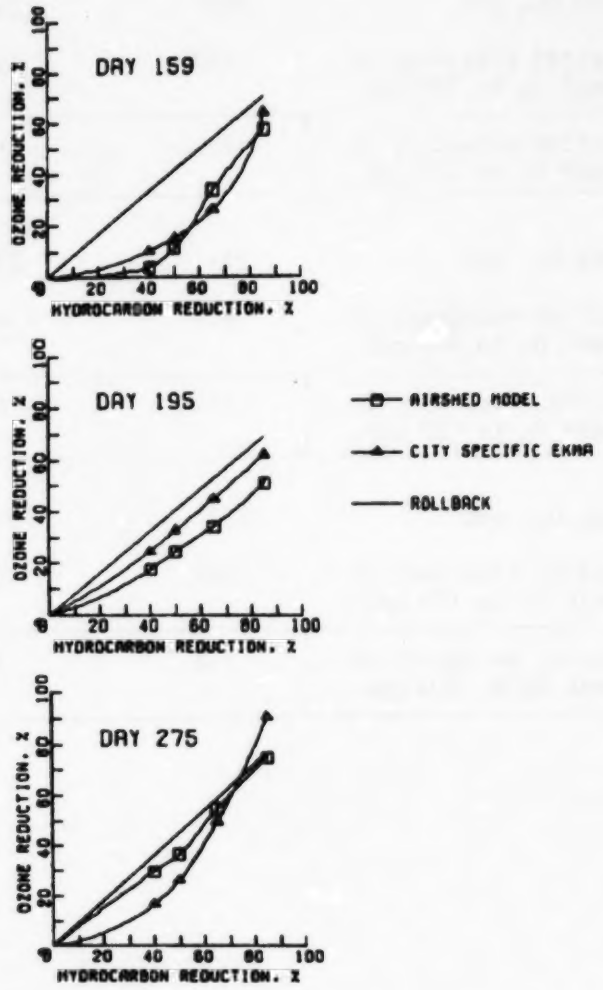

Figure 3-4. Comparison of Airshed, City-specific EKMA and Rollback to Changes in Hydrocarbons (High HC/NO_x Base Case).

Table 3-3. Emission Reductions Needed to Lower Peak O_3 to 120 ppb. (High HC/NO_x Conditions)

Day		Airshed	City-specific EKMA	Rollback
159	Base case O_3, ppb	325	325	325
	O_3 reduction necessary to lower peak O_3 to 120 ppb	63%	63%	63%
	HC reduction necessary to lower peak O_3 to 120 ppb	>85%	>85%	76%
195	Base case O_3, ppb	211	211	211
	O_3 reduction necessary to lower peak O_3 to 120 ppb	43%	43%	43%
	HC reduction necessary to lower peak O_3 to 120 ppb	75%	63%	53%
275	Base case O_3, ppb	331	331	331
	O_3 reduction necessary to lower peak O_3 to 120 ppb	64%	64%	64%
	HC reduction necessary to lower peak O_3 to 120 ppb	75%	73%	70%

Table 3-3. Emission Reductions Needed to Lower Peak O_3 to 120 ppb. (High HC/NO_x Conditions)

Day		Airshed	City-specific EKMA	Rollback
159	Base case O_3, ppb	325	325	325
	O_3 reduction necessary to lower peak O_3 to 120 ppb	63%	63%	63%
	HC reduction necessary to lower peak O_3 to 120 ppb	>85%	>85%	76%
195	Base case O_3, ppb	211	211	211
	O_3 reduction necessary to lower peak O_3 to 120 ppb	43%	43%	43%
	HC reduction necessary to lower peak O_3 to 120 ppb	75%	63%	53%
275	Base case O_3, ppb	331	331	331
	O_3 reduction necessary to lower peak O_3 to 120 ppb	64%	64%	64%
	HC reduction necessary to lower peak O_3 to 120 ppb	75%	73%	70%

Before describing the results, recall from Section 2.4 that control strategy predictions obtained with the Airshed Model did not deviate substantially from interpolated uniform emission reductions (see Figure 2-9). Furthermore, comparison of the simple models with Airshed Model in simulating the effectiveness of these more realistic strategies will necessarily focus on predictions in the intermediate range of hydrocarbon reductions (i.e., 22% to 56%). Thus, the results can be anticipated to some extent from previous discussions (primarily Section 3.3). Many of the same conclusions will hold, although numerical differences may occur.

Comparisons of the three models are depicted graphically in Figures 3-5 and 3-6. In each figure, the change in O_3 from the base case is plotted for each day, with Airshed predictions on the abcissa and the simple model on the ordinate. (City-specific EKMA is shown on the left and Rollback on the right.) The diagonal line represents perfect agreement. Points that lie above the line indicate that the simple model overestimates the effectiveness of a control program (using Airshed as the standard) and vice versa. Stated another way, points lying above the diagonal line would indicate that the simple model results in too much "credit" being given to the control program. In Figure 3-5, the independent model applications are shown. For the RACT strategy, both models tend toward an overestimation of the effectiveness of the program. For FMVECP, City-specific EKMA underestimates the effectiveness in all cases, although only slightly in two. Rollback agrees very well in two, and overestimates the effectiveness in another. The results are somewhat similar for the combined strategy. Rollback agrees very well in two cases, but overestimates the change in the third. City-specific EKMA agrees relatively well in two cases, and underestimates effectiveness in the third. Figure 3-6 presents the results when the models are put on a common basis. The same general conclusions hold as for the independent tests.

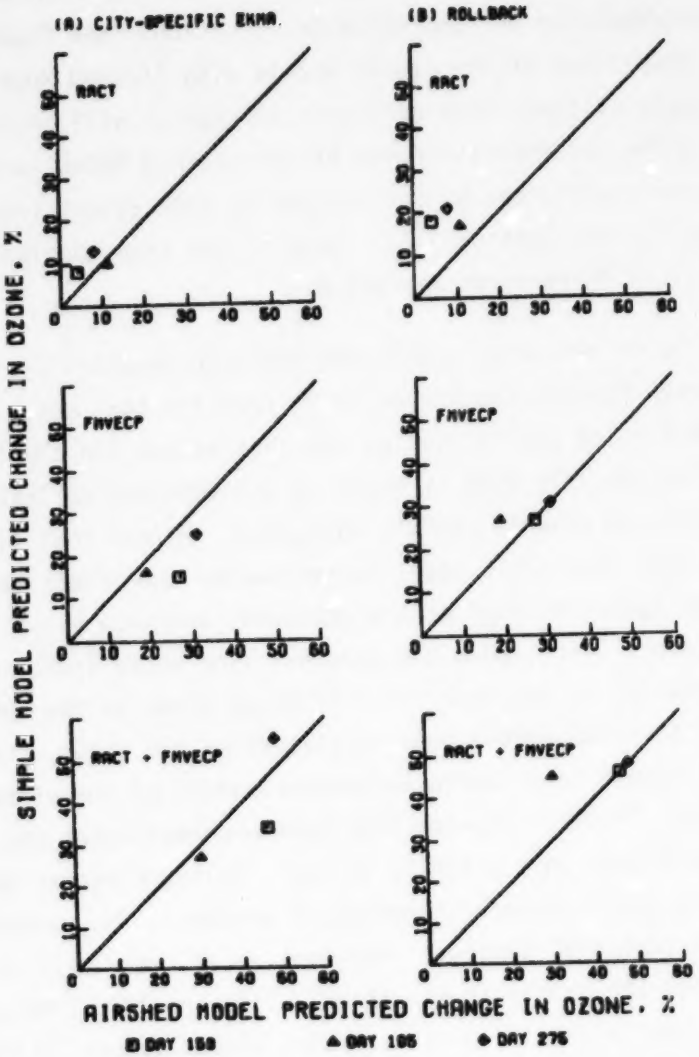

Figure 3-5. Comparison of Model Effectiveness Predictions for Control Strategies (Independent Tests).

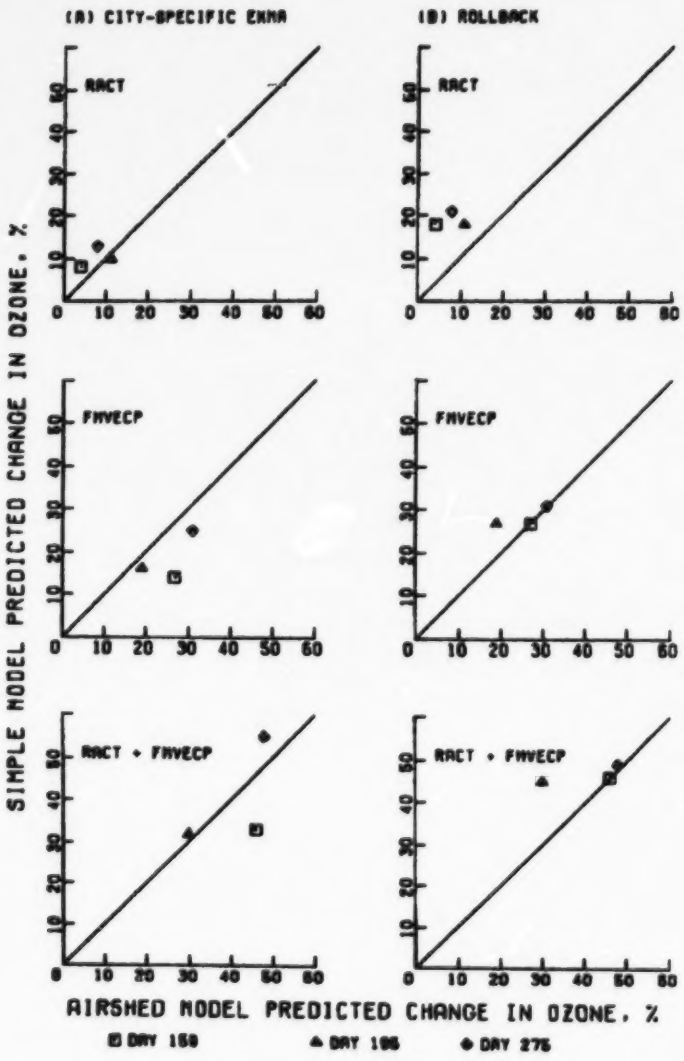

Figure 3-6. Comparison of Model Effectiveness Predictions for Control Strategies (Common Basis Tests).

4.0 CONCLUSIONS AND RECOMMENDATIONS

As set forth in the introduction, the primary purpose of this study has been to compare control effectiveness predictions of two simple models with those of a more complex PAQSM. Presumably, the more complex model should provide the best estimate because of its greater capacity for mathematically depicting the phenomena of ozone formation. Nevertheless, no guarantee exists that the PAQSM will provide accurate estimates of the effectiveness of reducing hydrocarbon emissions in lowering peak ozone levels. Though this problem cannot be circumvented, the PAQSM should be able to reproduce existing ozone patterns in order to mitigate to some extent the possibility of errors in the input data. Provided this criterion is met, the PAQSM can serve as one means of evaluating the simpler models ability to estimate the effectiveness of control programs.

A rudimentary analysis of the Airshed Model's predictions of ozone indicated that, in general, the predictions of peak ozone are within $\pm$30% of observations. However, isolated differences outside this range were indicated. Of the three days examined, the bias in the Airshed Model predictions tended towards underprediction of high ozone levels, although individual exceptions were noted. In one instance, the Airshed Model predicted the highest ozone concentration in an area in which no ozone monitor was located. While this prediction could obviously not be verified with observed data, it illustrates the value of such a model in assessing the regional nature of an ozone problem, and emphasizes the limitations of the simpler models.

The Airshed Model simulation of changes in hydrocarbons clearly demonstrates the potential of this type model for evaluating relative changes in ozone from base case levels. However, relating these results to typical regulatory applications is not a straightforward procedure. First of all, the Airshed Model simulations demonstrate that control programs may be more effective under certain meteorological conditions than for others, even though high ozone levels are found under each. These findings imply some potential problems in relating Airshed Model simulation results to the statistical form of the ozone standard. Secondly, techniques for incorporating any Airshed Model bias into regulatory analyses need further examination. Finally, in what may be a

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somewhat surprising finding, the limited number of Airshed Model simulations considered in this study indicated that the spatial, temporal and reactivity effects of particular control strategies may not be critical when compared to the impact of across-the-board, uniform emission reductions. That is, the ozone problem is more regional in nature, and does not appear to be significantly affected by microscale phenomena.

Comparisons of the simple models with the Airshed Model were complicated by differences in their mode of application and the form of the output typically available from each. Considering all of the tests, neither City-specific EKMA nor Rollback adequately reproduced the predictions of the Airshed Model over all conditions. Similarly, neither model was consistently overly or underly conservative in the predictions of the effectiveness of control programs in all situations. In other words, the findings did not indicate the superiority of either model in reproducing all Airshed Model results.

When model estimates of the degree of control required to reduce peak ozone levels to 120 ppb were made, the results again were mixed. However, in most instances, the differences in control estimates predicted by the Airshed Model and City-specific EKMA were about 10% or less, with City-specific EKMA giving the lower control estimate in practically every case. Some investigators have suggested that use of City-specific EKMA may result in overly conservative control estimates (i.e., estimating control levels that would result in overkill).[14,15] This suggestion is not supported by the results of this study. In fact, based on the Airshed Model results, City-specific EKMA may underestimate slightly the level of control needed to reduce peak ozone to 120 ppb. On the other hand, Rollback agreed with Airshed very well in some instances, but estimated much lower controls in other cases. In these cases, the difference in controls could be as much as 20%. Thus, Rollback is not overly conservative, but could lead to significant underpredictions of needed controls in some cases, especially at higher HC/NO_x ratios.

The above findings clearly demonstrate that the use of simple models can lead to different results than those obtained by using a PAQSM. Investigations are needed to unravel the reasons for these differences. While little

can be done in examining the Rollback model, further studies of the differences between Airshed and City-specific EKMA can be performed. Specifically, the following are recommended:

° Airshed and City-specific EKMA contain two different chemical mechanisms. Whether this difference is contributing significantly to the model discrepancies needs to be established.

° The relative importance of boundary conditions in each model needs closer scrutiny.

° City-specific EKMA should be compared to a more complex trajectory model which in turn should be compared to a PAQSM. Differences in the treatment of specific physical phenomena should be identified and their effect isolated to determine potential limitations with the City-specific EKMA technique.

° The comparisons conducted for the three days suggest that it will be difficult to generalize about the relationships between the simple models and the more complex PAQSMs. However, more days should be evaluated to discern apparent trends.

° Tests such as the ones described in this report need to be conducted for other cities to corroborate these findings.

° Further investigations are needed to establish the importance of NO_x in the Airshed Model versus City-specific EKMA.

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